



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:19 am BST

PDB ID : 4LL9  
Title : Crystal structure of D3D4 domain of the LILRB1 molecule  
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Deposited on : 2013-07-09  
Resolution : 2.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

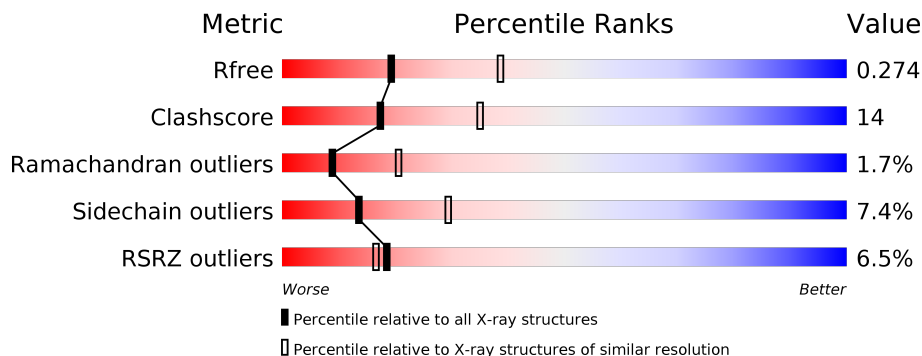
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	196	
1	B	196	
1	C	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	204	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1490	939	253	292	6	0	0	0
1	B	196	1499	944	255	294	6	0	0	0
1	C	196	1499	944	255	294	6	0	0	0

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	I	0	0
			4	4		
2	A	5	Total	I	0	0
			5	5		
2	C	3	Total	I	0	0
			3	3		

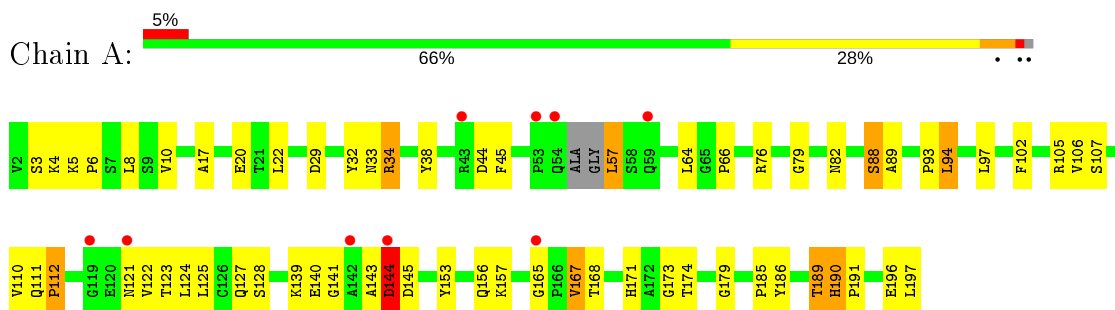
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	31	Total	O	0	0
			31	31		
3	C	24	Total	O	0	0
			24	24		

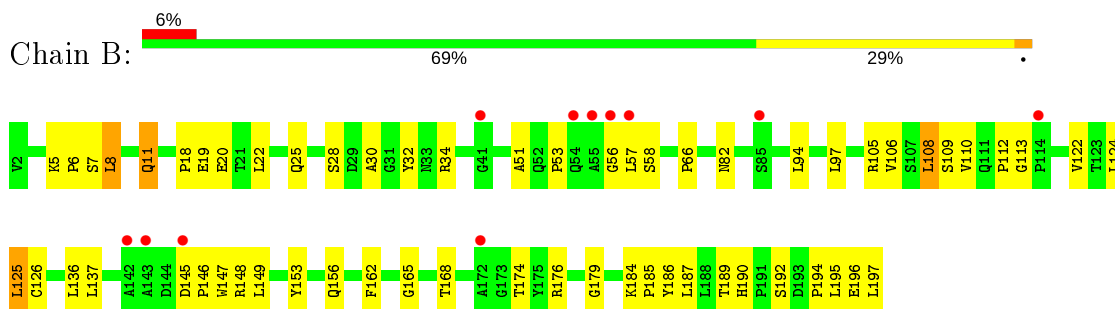
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

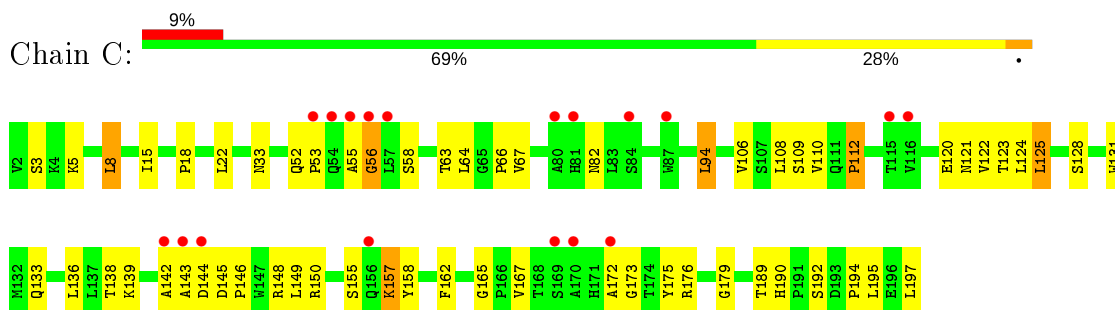
- Molecule 1: Leukocyte immunoglobulin-like receptor subfamily B member 1



- Molecule 1: Leukocyte immunoglobulin-like receptor subfamily B member 1



- Molecule 1: Leukocyte immunoglobulin-like receptor subfamily B member 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.26Å 71.98Å 75.04Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	32.81 – 2.69 32.81 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.81-2.69) 97.3 (32.81-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.68Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.245 , 0.275 0.245 , 0.274	Depositor DCC
$R_{free}$ test set	890 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtrriage
Anisotropy	0.523	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 37.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/1530	0.61	1/2084 (0.0%)
1	B	0.31	0/1540	0.59	1/2099 (0.0%)
1	C	0.31	0/1540	0.59	1/2099 (0.0%)
All	All	0.30	0/4610	0.60	3/6282 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	GLY	N-CA-C	6.22	128.66	113.10
1	B	11	GLN	C-N-CD	5.77	140.51	128.40
1	A	144	ASP	N-CA-C	5.37	125.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ALA	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1490	0	1419	44	0
1	B	1499	0	1428	40	0
1	C	1499	0	1428	40	1
2	A	5	0	0	4	0
2	B	4	0	0	1	0
2	C	3	0	0	0	0
3	A	35	0	0	6	0
3	B	31	0	0	6	0
3	C	24	0	0	6	0
All	All	4590	0	4275	121	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLN:OE1	1:B:25:GLN:NE2	2.14	0.80
1:C:143:ALA:HB1	1:C:144:ASP:HA	1.65	0.78
1:C:133:GLN:NE2	3:C:307:HOH:O	2.19	0.76
1:B:165:GLY:O	3:B:313:HOH:O	2.04	0.75
1:C:179:GLY:H	1:C:189:THR:HG22	1.50	0.74
1:A:179:GLY:H	1:A:189:THR:HG22	1.51	0.74
1:A:167:VAL:CG2	1:A:171:HIS:ND1	2.49	0.74
1:C:155:SER:HB2	1:C:157:LYS:HD3	1.71	0.72
1:A:167:VAL:HG23	1:A:171:HIS:ND1	2.05	0.72
1:B:19:GLU:OE2	1:C:150:ARG:NH1	2.23	0.71
1:B:179:GLY:H	1:B:189:THR:HG22	1.55	0.70
1:C:157:LYS:HG2	1:C:157:LYS:O	1.92	0.70
1:C:112:PRO:HD2	1:C:122:VAL:HG12	1.76	0.66
1:C:8:LEU:HD22	1:C:94:LEU:HD12	1.77	0.66
1:A:3:SER:OG	1:A:32:TYR:OH	2.13	0.65
1:A:102:PHE:O	3:A:307:HOH:O	2.14	0.65
1:B:18:PRO:O	3:B:314:HOH:O	2.14	0.65
1:A:64:LEU:O	3:A:306:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:VAL:HG12	1:C:128:SER:HB3	1.80	0.64
1:A:173:GLY:O	3:A:308:HOH:O	2.15	0.63
1:B:56:GLY:O	3:B:309:HOH:O	2.14	0.63
1:B:174:THR:OG1	1:B:196:GLU:OE2	2.16	0.62
1:A:167:VAL:HG22	1:A:171:HIS:ND1	2.14	0.62
1:C:179:GLY:H	1:C:189:THR:CG2	2.12	0.62
1:A:97:LEU:HD22	1:A:186:TYR:HA	1.81	0.62
1:A:111:GLN:HB3	1:A:112:PRO:HD3	1.82	0.61
1:B:110:VAL:HA	1:B:124:LEU:HA	1.82	0.61
1:B:97:LEU:HD23	1:B:186:TYR:HA	1.81	0.61
1:B:136:LEU:HD21	1:B:148:ARG:HH21	1.65	0.60
1:C:172:ALA:HA	1:C:197:LEU:HB2	1.82	0.60
1:B:53:PRO:HB3	1:B:57:LEU:HB3	1.84	0.59
1:A:153:TYR:CZ	1:A:156:GLN:HA	2.38	0.59
1:A:4:LYS:HE2	2:A:205:IOD:I	2.73	0.59
1:C:176:ARG:HH21	1:C:194:PRO:HG3	1.68	0.58
1:A:38:TYR:CZ	1:A:45:PHE:HB3	2.39	0.58
1:B:153:TYR:CZ	1:B:156:GLN:HA	2.39	0.58
1:C:189:THR:HG23	1:C:190:HIS:O	2.03	0.57
1:A:112:PRO:HG2	1:A:122:VAL:HG12	1.87	0.57
1:A:168:THR:O	1:A:171:HIS:HB2	2.05	0.57
1:A:179:GLY:H	1:A:189:THR:CG2	2.16	0.57
1:C:110:VAL:HA	1:C:124:LEU:HA	1.87	0.56
1:A:196:GLU:HA	3:A:308:HOH:O	2.06	0.55
1:B:124:LEU:HD12	1:B:162:PHE:HB2	1.87	0.55
1:B:106:VAL:HG23	1:B:192:SER:HB3	1.87	0.55
1:B:176:ARG:HE	1:B:194:PRO:HG3	1.71	0.55
1:C:106:VAL:HG23	1:C:192:SER:HB3	1.89	0.55
1:B:112:PRO:HD2	1:B:122:VAL:HG12	1.87	0.54
1:A:185:PRO:HD2	2:A:202:IOD:I	2.77	0.54
1:A:139:LYS:O	1:A:141:GLY:N	2.41	0.54
1:B:108:LEU:HD13	1:B:195:LEU:HB2	1.90	0.53
1:C:139:LYS:HD2	1:C:173:GLY:HA3	1.91	0.53
1:A:189:THR:HG23	1:A:190:HIS:O	2.09	0.52
1:A:157:LYS:NZ	3:A:319:HOH:O	2.41	0.52
1:B:53:PRO:HG3	1:B:58:SER:H	1.75	0.52
1:B:189:THR:HG23	1:B:190:HIS:O	2.09	0.52
1:C:5:LYS:O	3:C:303:HOH:O	2.19	0.52
1:A:105:ARG:CZ	1:B:145:ASP:HB3	2.40	0.52
1:B:147:TRP:NE1	1:B:149:LEU:HD13	2.26	0.51
1:A:29:ASP:HA	1:A:57:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:VAL:HG13	1:B:189:THR:HG21	1.93	0.51
1:A:190:HIS:HD2	3:A:307:HOH:O	1.94	0.51
1:C:149:LEU:HB2	1:C:162:PHE:CE1	2.45	0.51
1:B:179:GLY:H	1:B:189:THR:CG2	2.21	0.50
1:B:105:ARG:CZ	1:C:145:ASP:HB3	2.41	0.50
1:A:88:SER:OG	1:A:89:ALA:N	2.44	0.49
1:B:122:VAL:HG22	3:B:313:HOH:O	2.12	0.49
1:A:6:PRO:HD3	1:A:88:SER:OG	2.12	0.49
1:C:139:LYS:HB3	1:C:142:ALA:HB3	1.95	0.49
1:C:52:GLN:HG3	1:C:58:SER:HA	1.95	0.49
1:A:127:GLN:HB3	1:A:157:LYS:HE3	1.95	0.49
1:A:33:ASN:ND2	1:A:82:ASN:HA	2.28	0.48
1:A:29:ASP:HB3	1:A:57:LEU:HD23	1.96	0.48
1:A:76:ARG:CZ	1:A:93:PRO:HG3	2.44	0.47
1:C:120:GLU:H	1:C:167:VAL:HG12	1.79	0.47
1:A:139:LYS:HE3	1:A:173:GLY:HA3	1.97	0.47
1:A:33:ASN:OD1	1:A:34:ARG:HG2	2.15	0.47
1:A:110:VAL:HA	1:A:124:LEU:HA	1.97	0.47
1:C:55:ALA:HA	1:C:56:GLY:HA2	1.74	0.46
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.84	0.46
1:C:15:ILE:HD12	1:C:138:THR:HG21	1.98	0.46
1:A:106:VAL:HG12	1:A:128:SER:HB3	1.98	0.46
1:B:185:PRO:HD2	2:B:202:IOD:I	2.86	0.46
1:C:33:ASN:ND2	1:C:82:ASN:HA	2.31	0.46
1:A:79:GLY:H	1:A:88:SER:HB3	1.81	0.46
1:C:143:ALA:HB3	3:C:317:HOH:O	2.16	0.45
1:C:121:ASN:HA	1:C:165:GLY:O	2.16	0.45
1:C:109:SER:O	1:C:125:LEU:N	2.43	0.45
1:B:20:GLU:HG2	3:B:314:HOH:O	2.16	0.45
1:C:121:ASN:ND2	3:C:314:HOH:O	2.49	0.45
1:B:125:LEU:HD22	1:B:126:CYS:H	1.81	0.45
1:A:190:HIS:CE1	2:A:204:IOD:I	3.40	0.45
1:B:109:SER:O	1:B:125:LEU:N	2.40	0.45
1:B:5:LYS:HA	1:B:6:PRO:HD3	1.85	0.45
1:C:172:ALA:HA	1:C:197:LEU:CB	2.47	0.44
1:B:18:PRO:O	1:B:19:GLU:HB2	2.17	0.44
1:B:105:ARG:HG3	3:B:304:HOH:O	2.18	0.44
1:B:30:ALA:HB3	1:B:32:TYR:CE2	2.53	0.43
1:C:121:ASN:ND2	3:C:321:HOH:O	2.50	0.43
1:C:124:LEU:HD12	1:C:162:PHE:HB2	1.99	0.43
1:C:157:LYS:N	3:C:310:HOH:O	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HA	1:A:6:PRO:HD3	1.87	0.43
1:B:137:LEU:O	1:B:146:PRO:HB3	2.19	0.43
1:C:131:TRP:HD1	1:C:158:TYR:CZ	2.36	0.43
1:B:53:PRO:HB2	1:B:57:LEU:H	1.84	0.43
1:C:176:ARG:NH2	1:C:194:PRO:HG3	2.33	0.42
1:A:121:ASN:HA	1:A:165:GLY:O	2.20	0.42
1:C:175:TYR:O	1:C:194:PRO:HA	2.19	0.42
1:C:136:LEU:HD11	1:C:148:ARG:NE	2.34	0.42
1:B:28:SER:O	1:B:58:SER:HB3	2.20	0.42
1:B:124:LEU:HD11	1:B:137:LEU:HD22	2.01	0.42
1:A:167:VAL:HG22	1:A:171:HIS:CG	2.55	0.42
1:C:18:PRO:HA	1:C:67:VAL:HG23	2.02	0.42
1:C:145:ASP:HA	1:C:146:PRO:HD3	1.83	0.41
1:B:51:ALA:C	1:B:53:PRO:HD3	2.41	0.41
1:A:17:ALA:O	1:A:20:GLU:HB2	2.20	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.93	0.41
1:A:111:GLN:HB3	1:A:112:PRO:CD	2.50	0.41
1:C:149:LEU:HD12	1:C:149:LEU:HA	1.83	0.41
1:B:184:LYS:HB3	1:B:187:LEU:HD22	2.03	0.41
1:A:191:PRO:HD2	2:A:204:IOD:I	2.91	0.40
1:B:8:LEU:HD23	1:B:8:LEU:HA	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:THR:OG1	1:C:63:THR:OG1[2_556]	2.04	0.16

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/196 (97%)	178 (94%)	7 (4%)	5 (3%)	5	11
1	B	194/196 (99%)	177 (91%)	15 (8%)	2 (1%)	15	34
1	C	194/196 (99%)	180 (93%)	11 (6%)	3 (2%)	10	23
All	All	578/588 (98%)	535 (93%)	33 (6%)	10 (2%)	9	20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	112	PRO
1	B	66	PRO
1	C	66	PRO
1	A	145	ASP
1	C	53	PRO
1	A	140	GLU
1	A	144	ASP
1	B	113	GLY
1	C	112	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	146 (90%)	16 (10%)	8	16
1	B	162/163 (99%)	152 (94%)	10 (6%)	18	38
1	C	162/163 (99%)	152 (94%)	10 (6%)	18	38
All	All	486/489 (99%)	450 (93%)	36 (7%)	13	29

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	10	VAL
1	A	22	LEU

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Mol	Chain	Res	Type
1	A	34	ARG
1	A	44	ASP
1	A	57	LEU
1	A	88	SER
1	A	94	LEU
1	A	107	SER
1	A	123	THR
1	A	125	LEU
1	A	144	ASP
1	A	167	VAL
1	A	174	THR
1	A	189	THR
1	A	190	HIS
1	B	7	SER
1	B	8	LEU
1	B	22	LEU
1	B	34	ARG
1	B	82	ASN
1	B	94	LEU
1	B	108	LEU
1	B	125	LEU
1	B	168	THR
1	B	197	LEU
1	C	3	SER
1	C	8	LEU
1	C	22	LEU
1	C	64	LEU
1	C	94	LEU
1	C	108	LEU
1	C	123	THR
1	C	125	LEU
1	C	157	LYS
1	C	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	194/196 (98%)	0.18	9 (4%) 32 30	26, 65, 127, 190	0
1	B	196/196 (100%)	0.09	11 (5%) 24 22	25, 53, 104, 205	0
1	C	196/196 (100%)	0.52	18 (9%) 9 7	33, 75, 150, 214	0
All	All	586/588 (99%)	0.27	38 (6%) 18 16	25, 64, 134, 214	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	9.1
1	B	54	GLN	8.6
1	C	56	GLY	7.1
1	C	53	PRO	6.1
1	C	142	ALA	6.0
1	A	142	ALA	5.4
1	B	145	ASP	5.2
1	B	142	ALA	4.7
1	C	87	TRP	4.4
1	B	56	GLY	4.2
1	C	54	GLN	4.0
1	A	144	ASP	3.7
1	C	172	ALA	3.4
1	A	53	PRO	3.3
1	B	172	ALA	3.3
1	C	143	ALA	3.3
1	A	165	GLY	3.1
1	C	57	LEU	3.0
1	C	80	ALA	3.0
1	A	54	GLN	2.8
1	C	116	VAL	2.7
1	C	144	ASP	2.7
1	B	41	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	170	ALA	2.6
1	B	57	LEU	2.6
1	A	121	ASN	2.5
1	B	55	ALA	2.5
1	C	156	GLN	2.3
1	C	169	SER	2.3
1	B	114	PRO	2.3
1	C	81	HIS	2.2
1	A	119	GLY	2.2
1	C	84	SER	2.1
1	A	59	GLN	2.1
1	B	143	ALA	2.1
1	A	43	ARG	2.1
1	C	115	THR	2.1
1	B	85	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IOD	B	204	1/1	0.58	0.10	159,159,159,159	1
2	IOD	C	203	1/1	0.90	0.08	115,115,115,115	0
2	IOD	A	205	1/1	0.91	0.07	145,145,145,145	0
2	IOD	C	201	1/1	0.98	0.07	81,81,81,81	0
2	IOD	B	203	1/1	0.99	0.04	70,70,70,70	0
2	IOD	A	204	1/1	0.99	0.07	61,61,61,61	0
2	IOD	A	202	1/1	0.99	0.07	59,59,59,59	0
2	IOD	A	201	1/1	0.99	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	C	202	1/1	0.99	0.03	90,90,90,90	0
2	IOD	B	201	1/1	1.00	0.11	52,52,52,52	0
2	IOD	A	203	1/1	1.00	0.10	50,50,50,50	0
2	IOD	B	202	1/1	1.00	0.07	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.